



**3rd MAGICS Workshop, Nov. 11 – 13, 2018 at Gaithersburg Marriott
Washingtonian Center, Gaithersburg, MD**

WORKSHOP AGENDA

Sunday, November 11, 2018

Time	Event
11:00 am–12:00 pm	Registration
12:00 pm – 1:30 pm	Lunch and Registration
1:30 – 2:30 pm	HPC Account Setup for all participants
2:30 – 2:45 pm	Introduction to MAGICS workshop Priya Vashishta
2:45 – 3:30 pm	Lecture: Introduction to molecular dynamics and thermal conductivity computation Instructor: Priya Vashishta, USC
3:30 – 4:30 pm	Hands-on: Thermal conductivity plugin download and set up. Instructor: Aravind Krishnamoorthy, Pankaj Rajak, Ankit Mishra, Nitish Baradwaj, Nick Grabar, USC
4.30 – 5.00 pm	Break
5:00 – 6:30 pm	Hands-on: Thermal conductivity computation and visualization Instructor: Aravind Krishnamoorthy, Pankaj Rajak, Nitish Baradwaj, Ankit Mishra, Nick Grabar, USC
6:30 – 8.00 pm	Reception and Dinner

Monday, November 12, 2018

Time	Event
7:30 – 8:15 am	Breakfast
8:30 – 8:45 am	Overview of the Day
8:45 – 9:45 am	Lecture: Reactive Force Field (ReaxFF) Instructors: Sungwook Hong, Ken-ichi Nomura, USC
9:45 – 10:45 am	Hands-on: RXMD Software Introduction Instructors: Ken-ichi Nomura, Sungwook Hong, Ankit Mishra, Ruru Ma, Subodh Tiwari, USC
10:45 – 11:00 am	Break
11:00 – 12:30 pm	Hands-on: RXMD Software Hands on I Instructors: Ken-ichi Nomura, Sungwook Hong, Ankit Mishra, Ruru Ma, Subodh Tiwari, USC
12:30 – 1:30 pm	Lunch
2:00 pm – 3:00 pm	Lecture and Demonstration: Materials Project Instructors: Kristin Persson, LBNL and UC Berkeley
3:00 – 4:00 pm	Hands-on: RXMD Software Hands on II Instructors: Ken-ichi Nomura, Sungwook Hong, Ankit Mishra, Ruru Ma, Subodh Tiwari, USC
4:00 – 4:30 pm	Break
4:30 – 6:00 pm	Hands-on: RXMD Software Hands on II-Continued Instructors: Ken-ichi Nomura, Sungwook Hong, Ankit Mishra, Ruru Ma, Subodh Tiwari, USC
6:30 – 8:00 pm	Dinner/Banquet

Tuesday, November 13, 2018

Time	Event
7:30 – 8:15 am	Breakfast
8:15 – 8:30 pm	Overview of the Day
8:30 – 9:30 pm	Lecture: Quantum Molecular Dynamics Instructor: Aiichiro Nakano, USC
9:30 – 10:15 am	Lecture: Introduction to QXMD Software Instructor: Subodh Tiwari, Aravind Krishnamoorthy, Lindsay Bassman, Ken-ichi Nomura, USC
10:15 – 10:45 am	Break
10:45 – 11:30 am	Hands-on: QXMD Software Hands on I Instructor: Subodh Tiwari, Aravind Krishnamoorthy, Lindsay Bassman, Ken-ichi Nomura USC
11:30 – 12:30 pm	Hands-on: QXMD Software Hands on I - Continued Instructor: Subodh Tiwari, Aravind Krishnamoorthy, Lindsay Bassman, Ken-ichi Nomura USC
12:30 – 1:30 pm	Lunch and Discussion on Research Collaboration

2:00 – 2:30 pm	Lecture: Machine Learning in Materials Science Instructor: Rajiv K. Kalia, USC
2:30 – 3:30 pm	Demo: Machine Learning in Materials Science Instructor: Rajiv K. Kalia, Pankaj Rajak, Priya Vashishta, Kuang Liu, USC
3:30 – 4:00 pm	Break
4:00 – 5.00 pm	Demo: Dame-Engine Assisted Research platform for Scientific Computing (GEARS): Using virtual reality in visualizing simulations